1,3,5-Cycloheptatriene

544-25-2 | DTXSID5073909

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 10.2 days

Global applicability domain: Inside

Local applicability domain index: 4.38e-01

Confidence level: 6.95e-01

Nearest Neighbors from the Training Set

Image not found
Indan
Measured: 61.9
Predicted: 8.13

Image not found
1,2,3-Trimethylbenzene
Measured: 24.3
Predicted: 4.97

Image not found
1,1-Dimethylcyclopentane
Measured: 880
Predicted: 10.9

Image not found
1,2-Dimethylcyclohexane
Measured: 777
Predicted: 10.2

Image not found
Cumene
Measured: 511
Predicted: 11.8